5 Technology Roadmap

Workshop discussions in each of the four tracks produced a set of near-term, mid-term and long-term research needs to achieve the goal *that by 2015 multiphase science based computer simulations play a significant role in the design, operation, and troubleshooting of multiphase flow devices in fossil fuel processing plants.* These needs include further developments in theory, experiments, computational algorithm and code development and validation. The research needs in the four tracks were then put together in an effort to identify themes that cut across the various tracks. An initial presentation on such integration was prepared by Professors Dimitri Gidaspow and Sankaran Sundaresan. They observed that the workshop identified several issues that cut across the four tracks, which can be grouped into four categories:

- Numerical algorithm and software development
- Theory and model development
- Physical and computational experiments
- Communication, collaboration and education

The information from the four track reports is summarized below grouped into the above four categories and the category of benchmark cases identified during the work shop.

	Near-Term (by 2009)	Mid-Term (by 2012)	Long-Term (by 2015)
A. Benchmark Cases	1. High-fidelity, transient, 3-D, two-phase with PSD (no density variations), hydrodynamics-only simulation of transport reactor at TRDU-scale (200 kg/h coal feed rate) to run on 2009 computer cluster overnight. 2. Develop reduced-order, approximately real-time model of the above case that can be linked to process simulators.	1. High-fidelity, transient, 3-D, two-phase with PSD (no density variations), hydrodynamics with heat and mass transfer simulation of transport reactor at a scale of at least 12.5 MW (or 5,000 kg/h coal feed rate) to run on 2012 computer cluster overnight. 2. Repeat Near-Term Case 1 with addition of considering density variations (multiple solids species) 3. Develop reduced-order, approximately real-time models of Mid-Term Case 1 that can be linked to process simulators	1. High-fidelity, transient, 3-D, two-phase with particle size and density variations, hydrodynamics with chemical reactions simulation of transport reactor at a scale of at least 25 MW (or 10,000 kg/h coal feed rate) to run on 2015 computer cluster overnight. 2. Develop reduced-order, approximately real-time models of Long-Term Case 1 that can be linked to process simulators
B. Numerical Algorithm and Software Development	1. Improve numerical stability and efficiency of parallel computations. 2. Develop detailed protocol for the integration of various codes; e.g., Common component architecture for linking software components. 3. Develop coarse-grained (filtered) two-fluid models. 4. Develop reduced order models from accurate computational results for use by design engineers. 5. Demonstrate that the models correctly capture the effect of temperature and pressure.	1. Demonstrate that the models are able to predict the transition in the fluidization behavior when the particle properties change from Geldart group B to group A. 2. Develop initial fully coupled reactive multiphase flow model. 3. Develop automated procedure to coarsen hydrodynamic (non-reactive or with simple reactions) results from CFD for use with more complex reaction networks. 4. Develop in-situ adaptive tabulation of chemical reaction rates for heterogeneous reactions and couple with full CFD simulation for reactive	1. Integrate developments to complete fully coupled reactive flow model for industrial-scale reactors capable of handling a range of mesh sizes with reasonable run times. 2. Solve numerical stiffness problems in multi-physics simulations (reaction, radiation, density jumps, etc) 3. Demonstrate that models that can correctly model the effect of internals such as heat transfer tubes. 4. Investigate the use of the detailed models for scale up and process control (See Table 1.4).

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	6. Identify the deficiencies of the current models, assess the state-of-the-art, and document the "current best approach". 7. Identify a standard approach for multiphase flow code verification. 8. Develop a plan for generating validation test cases, identify fundamental experiments, and identify computational challenge problems.	flows. 5. Develop models and codes that explicitly recognize and account for the micro/meso/macroscale picture that is emerging from studies at these different scales. 6. Develop software framework that allows multiple codes (open-source and commercial) to work together. 7. Solve numerical issues with the treatment of PSD (e.g., DQMOM).	
C. Theory and Model Development	1. Develop fundamental aspects of stress and flow fields in dense particulate systems (See Table 1.1). 2. Develop drag relations that can handle particle size and density distributions and are applicable over the entire range of solids volume fraction. 3. Develop stress relations for dilute poly-disperse systems. 4. Formulate proper boundary conditions for multiphase flow systems. The wall boundary condition must capture key effects such as the solids flux distribution near a wall. Exits – how to handle solids versus	1. Develop continuum descriptions of dense particulate systems (See Table 1.3). 2. Handle the transition from regimes in which the particles are in enduring contact to regimes in which the particles are in collisional contact. 3. Develop methods to model adsorption/desorption and heterogeneous chemical reactions. 4. Determine the significance of electrostatic forces and van der Waals (cohesive) forces on hydrodynamics and develop appropriate models. 5. Develop the theory to model liquid feed injection and	1. Model particle deposition and re-suspension, which includes the effect of particle size distribution. 2. Model particle attrition and agglomeration, and fragmentation of coal. 3. Account for particle dispersion in solid-fuel injectors and gasifiers. We need to simultaneously account for particle dispersion as well as fluctuating kinetic energy. 4. Determine the significance of gas emanation from particles (via chemical reactions) on overall hydrodynamics and develop appropriate models. 5. Develop model for erosion of

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	gas boundary conditions. Use DEM or other techniques to resolve issues. 5. Understand the cause and effects of particle clustering. The effect of particle clustering on drag, collisions, and gas-phase turbulence modulation are needed. 6. Development of constitutive relations for continuum models from discrete models such as DEM or LBM, which are based on fewer assumptions than the continuum approach. 7. Identify flow-regimes in gas-liquid and gas-liquid-solids flows and develop appropriate constitutive relations and simplified models.	subsequent evaporation of liquids. 6. Model flow regime transitions in gas-liquid flows; e.g., the transition in a bubble column from "bubbly" to "churn turbulent" regime. 7. Develop radiation model for particle-particle and particle-wall heat transfer. 8. Develop constitutive models for non-spherical particles. 9. Develop multiphase turbulence models that incorporate fluctuations in the volume fraction. 10. Consider the effect of lubrication forces in particle-particle interactions.	walls or internals by particle impact. 6. Solve several fundamental theoretical challenges in mathematical formulations of multiphase flow: resolution of ill-posedness of continuum multiphase flow equations, eliminating the need to time-average the solution of continuum models for statistically steady problems.
D. Physical and Computational Experiments	1. Provide detailed circulating fluidized bed data on at least two scales (~0.15 m and ~0.6 m diameter vessels). The experiments must have well-defined entrance, exit, and boundary conditions and should report detailed data for local pressure, velocity of solids and gas, solids fraction, fluctuations, cluster sizes, and	1. Define material properties on relevant scales, along with efficient ways to represent properties in models and establish standards for material property measurements (See Table 1.2). 2. Use large flow facility to elucidate the effect of particle size distribution on flow. Determine lateral distribution of	1. Full-field visualizations of rotational motions of spherical and non-spherical particles in quasi-2-dimensional situations and 3-d tracking of particles in semi-dilute situations (volume fractions of up to 10 or 15%) that takes into account: frictional interactions, bidisperse or polydisperse grains, and non-

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	solids flux. 2. Develop well-calibrated, non-intrusive probes to simultaneously measure the velocity and volume fraction of different phases. Planar flow field, rather than point-to-point traverses, is required (e.g., measure radial solids concentration in riser using MRI). 3. Develop experimental techniques for gaining information from deep into opaque multiphase mixtures. 4. Measurements of near wall phenomena to establish wall boundary conditions. 5. Small-scale experiments to provide data to improve and check sub-models; e.g., simultaneously measure drag in gas-solids flows as well as gas and solid velocities (slip). 6. Develop standardized experiments or detailed simulations (discrete element or lattice Boltzmann) or a combination of both to derive a custom drag formula for a given powder.	particle sizes and segregation. 3. Measure spatial variation of PSD. 4. Conduct multiphase chemical reactor experiments with detailed measurements (e.g., ozone decomposition in fluidized beds). 5. Determine the importance of flow- generated electrostatic forces on dilute gas-solids flows for both cold and hot (process) conditions. 6. Measure flow fields in the presence of obstacles, such as heat transfer tubes, baffles, etc. 7. Develop measurement techniques for high pressure and temperature bubble columns. 8. Collect detailed data from 3-D tomography (MRI, X-ray, capacitance imaging etc.)	spherical grains.

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E. Communication, Collaboration, and Education	1. Constitute a task force to define benchmark gas-liquid and liquid-solids problems, which will guide CFD model development and experimental work. 2. Establish a communications network for the multiphase research community, which may include newsletter, web page, and regularly scheduled seminars and workshops. 3. Education: Develop curriculum for modular university courses; train adequate number of graduate students in this area; develop on-line instructional modules.	1. Establish communication between different entities working on open source multiphase flow codes. 2. Develop challenge problems for multiphase flow with heat & mass transfer and chemical reactions.	